



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 04:48 PM BST

PDB ID : 2IH9
Title : A high-dose crystal structure of a recombinant *Melanocarbonylase* lac-case
Authors : Hakulinen, N.; Rouvinen, J.
Deposited on : 2006-09-26
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

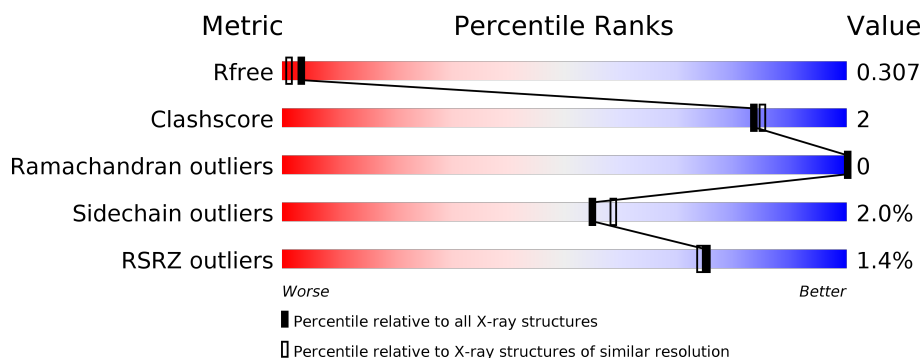
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




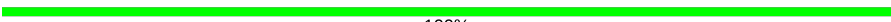
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	559	<div> <div>2%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
1	B	559	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>
2	C	3	<div> <div>67%</div> <div>33%</div> </div>
2	D	3	<div> <div>33%</div> <div>67%</div> </div>
2	F	3	<div> <div>67%</div> <div>33%</div> </div>
2	G	3	<div> <div>33%</div> <div>33%</div> <div>33%</div> </div>

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Mol	Chain	Length	Quality of chain
3	E	2	 50%50%
3	H	2	 100%

2 Entry composition [i](#)

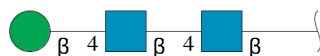
There are 8 unique types of molecules in this entry. The entry contains 9822 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Laccase-1.

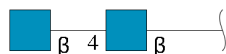
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	559	Total	C	N	O	S	0	0	0
			4369	2764	759	831	15			
1	B	559	Total	C	N	O	S	0	0	0
			4369	2764	759	831	15			

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

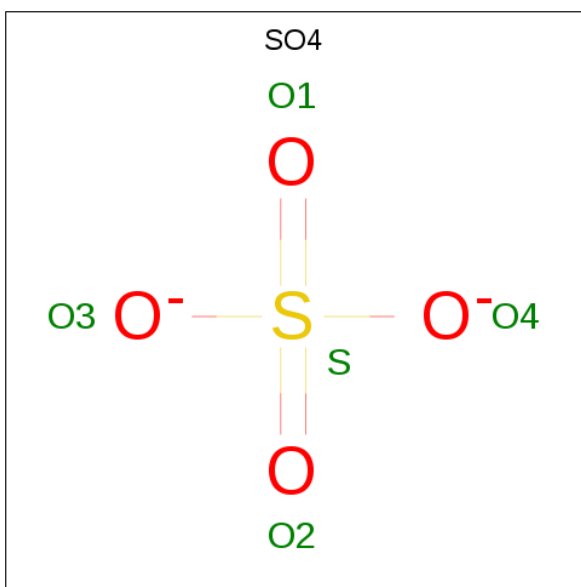
- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	4	Total	Cu	0	0
			4	4		
5	A	4	Total	Cu	0	0
			4	4		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		

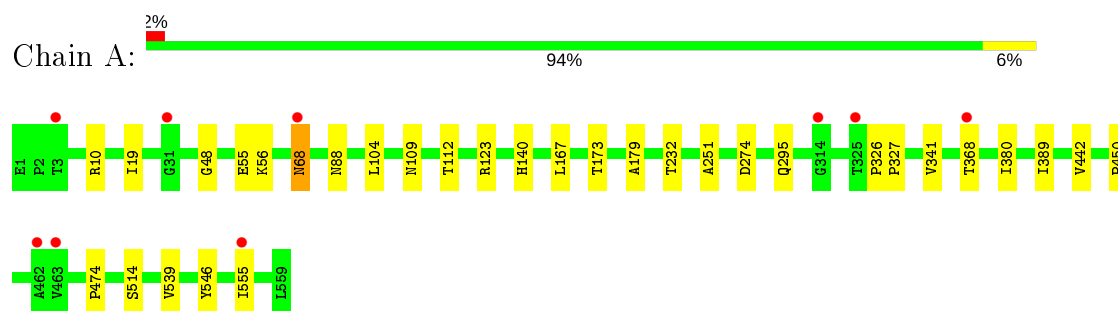
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	363	Total 363	O 363	0	0
8	B	344	Total 344	O 344	0	0

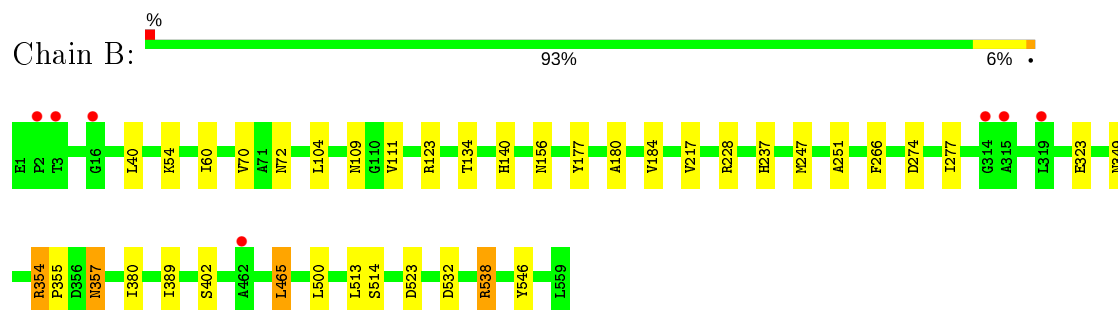
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

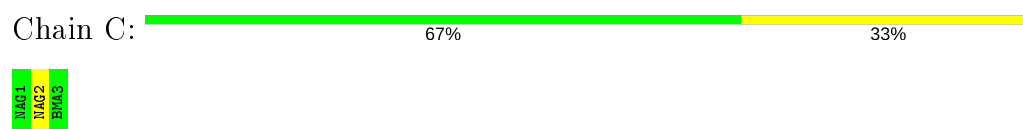
- Molecule 1: Laccase-1



- Molecule 1: Laccase-1



- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  67% 33%



- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  33% 33% 33%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.49 Å 62.33 Å 125.10 Å 90.00° 96.25° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 19.66 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (25.00-2.00) 99.5 (19.66-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.78 (at 2.01 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.263 , 0.299 0.274 , 0.307	Depositor DCC
R_{free} test set	4504 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.704	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9822	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, BMA, NAG, CU, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.67	0/4506	0.76	0/6191
1	B	0.66	0/4506	0.75	0/6191
All	All	0.66	0/9012	0.75	0/12382

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	546	TYR	Sidechain
1	B	546	TYR	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4369	0	4111	16	0
1	B	4369	0	4111	23	0
2	C	39	0	34	3	0
2	D	39	0	34	1	0
2	F	39	0	34	0	0
2	G	39	0	34	1	0
3	E	28	0	25	0	0
3	H	28	0	25	0	0
4	A	70	0	65	4	0
4	B	70	0	65	1	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	10	0	0	0	0
7	B	5	0	0	0	0
8	A	363	0	0	5	0
8	B	344	0	0	5	0
All	All	9822	0	8538	43	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (43) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:VAL:HG22	4:B:760:NAG:H81	1.35	1.04
4:A:720:NAG:H61	4:A:721:NAG:H82	1.49	0.93
1:A:104:LEU:HD21	1:A:389:ILE:HG21	1.64	0.79
1:B:323:GLU:OE2	2:G:2:NAG:H4	1.95	0.67
1:B:349:ASN:HA	1:B:465:LEU:HD11	1.78	0.65
1:B:104:LEU:HD12	1:B:532:ASP:HB3	1.81	0.61
1:A:167:LEU:O	4:A:760:NAG:H82	2.00	0.60
1:A:10:ARG:HG2	8:A:831:HOH:O	1.99	0.60
4:A:720:NAG:H61	4:A:721:NAG:C8	2.28	0.59
1:B:70:VAL:HG13	8:B:901:HOH:O	2.02	0.59
1:B:104:LEU:HD21	1:B:389:ILE:HG21	1.84	0.58
1:A:251:ALA:HB3	1:A:274:ASP:HB2	1.86	0.58
1:B:251:ALA:HB3	1:B:274:ASP:HB2	1.88	0.55
1:B:134:THR:HG23	8:B:1047:HOH:O	2.08	0.54
1:B:357:ASN:HD22	1:B:357:ASN:C	2.12	0.53
4:A:720:NAG:O4	4:A:721:NAG:C1	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:ILE:HG21	1:B:514:SER:HB3	1.90	0.52
1:A:179:ALA:CB	2:C:2:NAG:H81	2.41	0.51
1:A:380:ILE:HG21	1:A:514:SER:HB3	1.92	0.50
1:B:180:ALA:O	1:B:184:VAL:HG23	2.14	0.47
1:B:40:LEU:HD23	1:B:60:ILE:HG12	1.96	0.47
1:B:72:ASN:HD22	1:B:156:ASN:HB2	1.80	0.47
1:A:48:GLY:HA3	8:A:900:HOH:O	2.14	0.46
1:A:55:GLU:OE2	2:C:2:NAG:H83	2.16	0.45
1:A:19:ILE:HG13	1:A:341:VAL:HG11	1.99	0.45
1:B:54:LYS:HD2	1:B:177:TYR:HA	1.99	0.44
1:A:442:VAL:HB	1:A:474:PRO:HG2	2.00	0.43
1:B:40:LEU:CD2	1:B:60:ILE:HG12	2.48	0.43
1:B:228:ARG:HG2	1:B:274:ASP:OD1	2.19	0.43
1:B:355:PRO:HG3	8:B:1040:HOH:O	2.19	0.43
1:B:538:ARG:NH2	8:B:906:HOH:O	2.51	0.42
1:A:326:PRO:HA	1:A:327:PRO:HD3	1.96	0.42
1:B:354:ARG:H	1:B:357:ASN:HD21	1.67	0.42
1:A:539:VAL:HG11	8:A:1081:HOH:O	2.19	0.42
1:B:237:HIS:HB3	1:B:266:PHE:CZ	2.55	0.42
1:A:104:LEU:HD23	1:A:112:THR:O	2.19	0.41
1:A:68:ASN:HB2	8:A:1028:HOH:O	2.18	0.41
8:A:901:HOH:O	2:D:1:NAG:H83	2.20	0.41
1:A:56:LYS:HD2	2:C:2:NAG:H82	2.02	0.41
1:B:111:VAL:HG21	1:B:500:LEU:HD21	2.01	0.41
1:B:247:MET:HG2	1:B:277:ILE:HD13	2.03	0.41
1:A:173:THR:HB	1:A:232:THR:OG1	2.21	0.41
1:B:156:ASN:ND2	8:B:901:HOH:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	557/559 (100%)	538 (97%)	19 (3%)	0	100	100
1	B	557/559 (100%)	538 (97%)	19 (3%)	0	100	100
All	All	1114/1118 (100%)	1076 (97%)	38 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	478/478 (100%)	469 (98%)	9 (2%)	57	61
1	B	478/478 (100%)	468 (98%)	10 (2%)	53	57
All	All	956/956 (100%)	937 (98%)	19 (2%)	55	58

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	88	ASN
1	A	109	ASN
1	A	123	ARG
1	A	140	HIS
1	A	295	GLN
1	A	368	THR
1	A	450	PRO
1	A	555	ILE
1	B	109	ASN
1	B	123	ARG
1	B	140	HIS
1	B	354	ARG
1	B	357	ASN
1	B	402	SER
1	B	465	LEU
1	B	513	LEU
1	B	523	ASP

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Mol	Chain	Res	Type
1	B	538	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	45	ASN
1	A	72	ASN
1	A	99	GLN
1	A	144	GLN
1	A	213	GLN
1	A	236	ASN
1	A	244	ASN
1	A	413	GLN
1	B	72	ASN
1	B	99	GLN
1	B	144	GLN
1	B	295	GLN
1	B	357	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

16 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1	1,2	14,14,15	0.55	0	17,19,21	0.64	0
2	NAG	C	2	2	14,14,15	0.50	0	17,19,21	0.65	0
2	BMA	C	3	2	11,11,12	0.56	0	15,15,17	0.24	0
2	NAG	D	1	1,2	14,14,15	0.66	0	17,19,21	0.59	0
2	NAG	D	2	2	14,14,15	0.56	0	17,19,21	0.99	1 (5%)
2	BMA	D	3	2	11,11,12	0.55	0	15,15,17	0.28	0
3	NAG	E	1	1,3	14,14,15	0.61	0	17,19,21	0.62	0
3	NAG	E	2	3	14,14,15	0.55	0	17,19,21	0.66	1 (5%)
2	NAG	F	1	1,2	14,14,15	0.57	0	17,19,21	0.88	1 (5%)
2	NAG	F	2	2	14,14,15	0.49	0	17,19,21	0.62	0
2	BMA	F	3	2	11,11,12	0.51	0	15,15,17	0.26	0
2	NAG	G	1	1,2	14,14,15	0.57	0	17,19,21	0.61	0
2	NAG	G	2	2	14,14,15	0.75	0	17,19,21	1.39	2 (11%)
2	BMA	G	3	2	11,11,12	0.55	0	15,15,17	0.87	1 (6%)
3	NAG	H	1	1,3	14,14,15	0.55	0	17,19,21	0.75	0
3	NAG	H	2	3	14,14,15	0.58	0	17,19,21	0.63	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	1/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	BMA	G	3	2	-	0/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	NAG	C4-C3-C2	-4.05	105.08	111.02
2	G	3	BMA	C1-C2-C3	2.90	113.23	109.67
2	G	2	NAG	O4-C4-C3	2.64	116.46	110.35
2	F	1	NAG	C2-N2-C7	-2.13	119.87	122.90
3	E	2	NAG	C2-N2-C7	-2.06	119.97	122.90
2	D	2	NAG	C4-C3-C2	2.00	113.95	111.02

There are no chirality outliers.

All (17) torsion outliers are listed below:

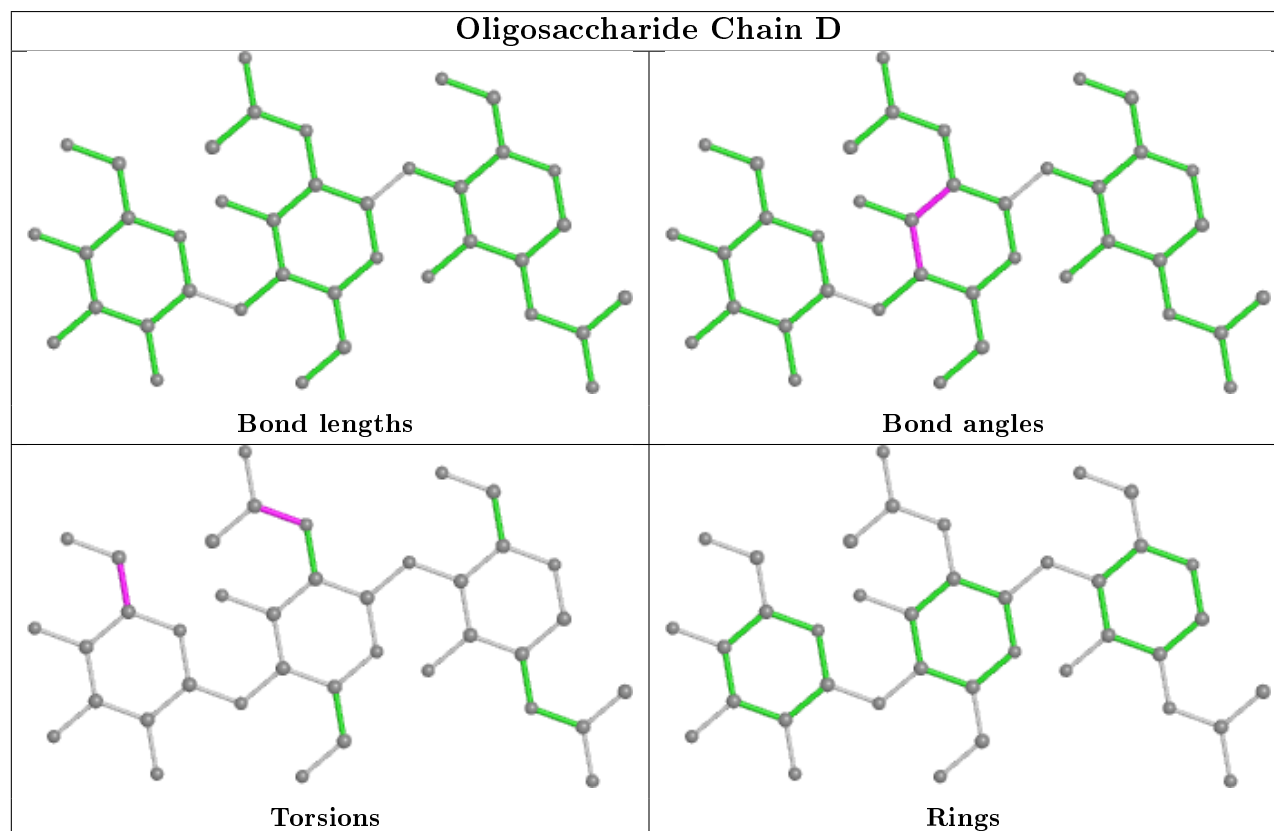
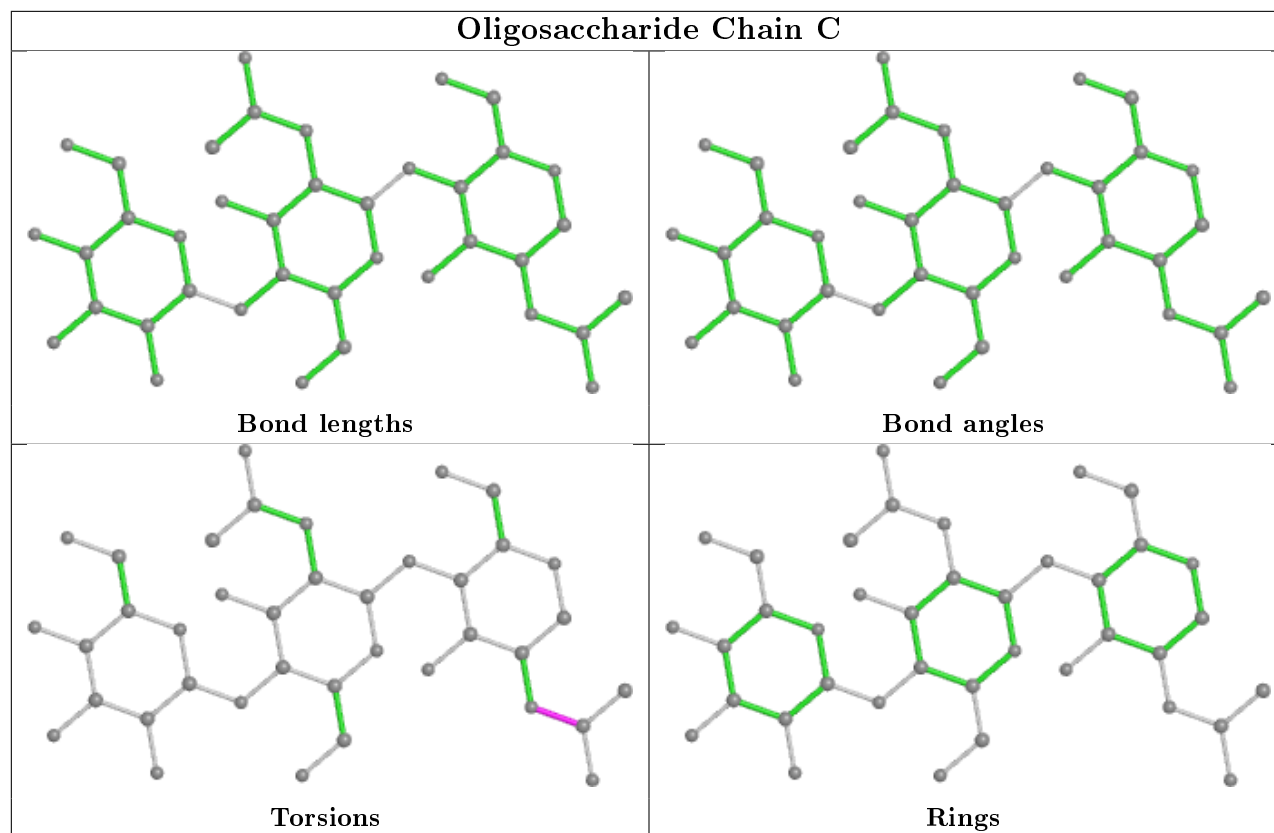
Mol	Chain	Res	Type	Atoms
3	H	2	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	H	2	NAG	C8-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O7-C7-N2-C2
3	E	1	NAG	O5-C5-C6-O6
3	E	1	NAG	O7-C7-N2-C2
2	D	3	BMA	O5-C5-C6-O6

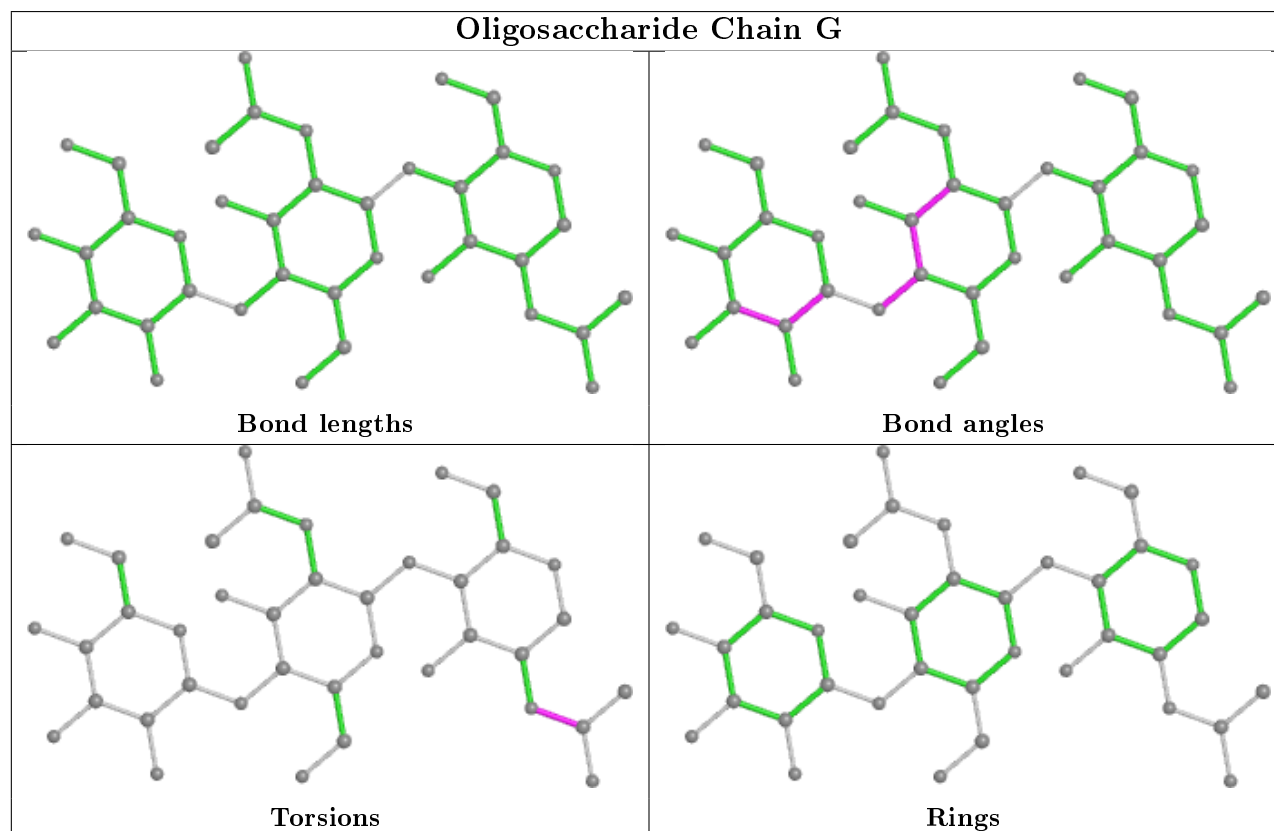
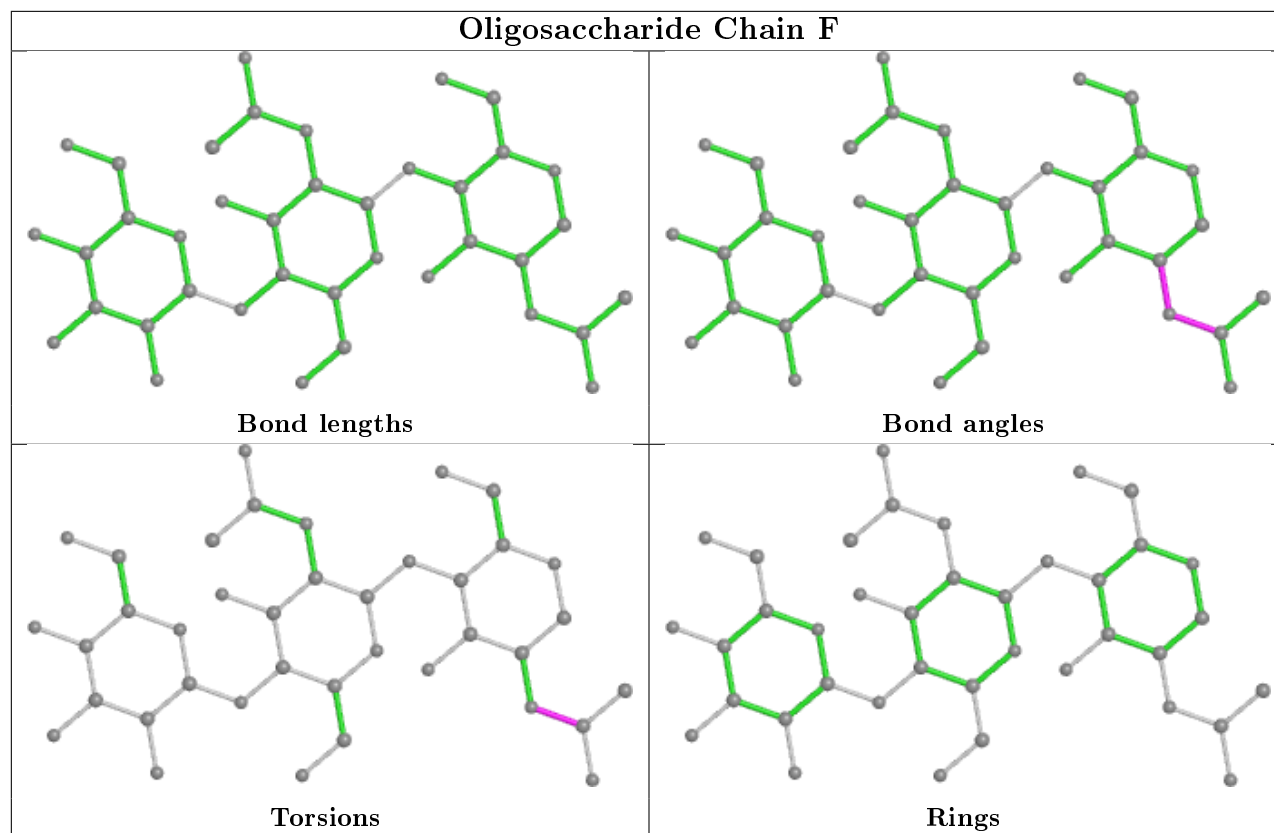
There are no ring outliers.

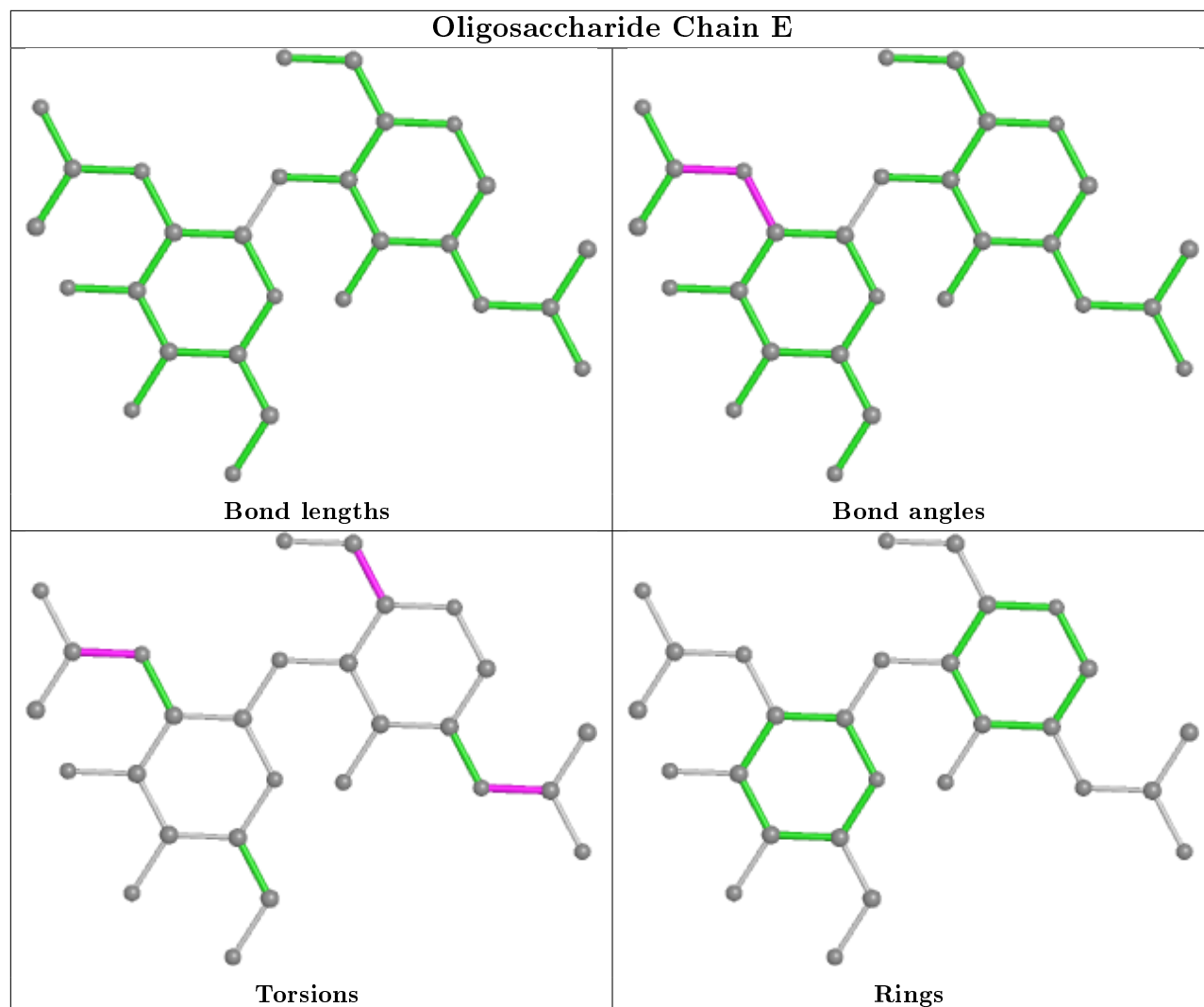
3 monomers are involved in 5 short contacts:

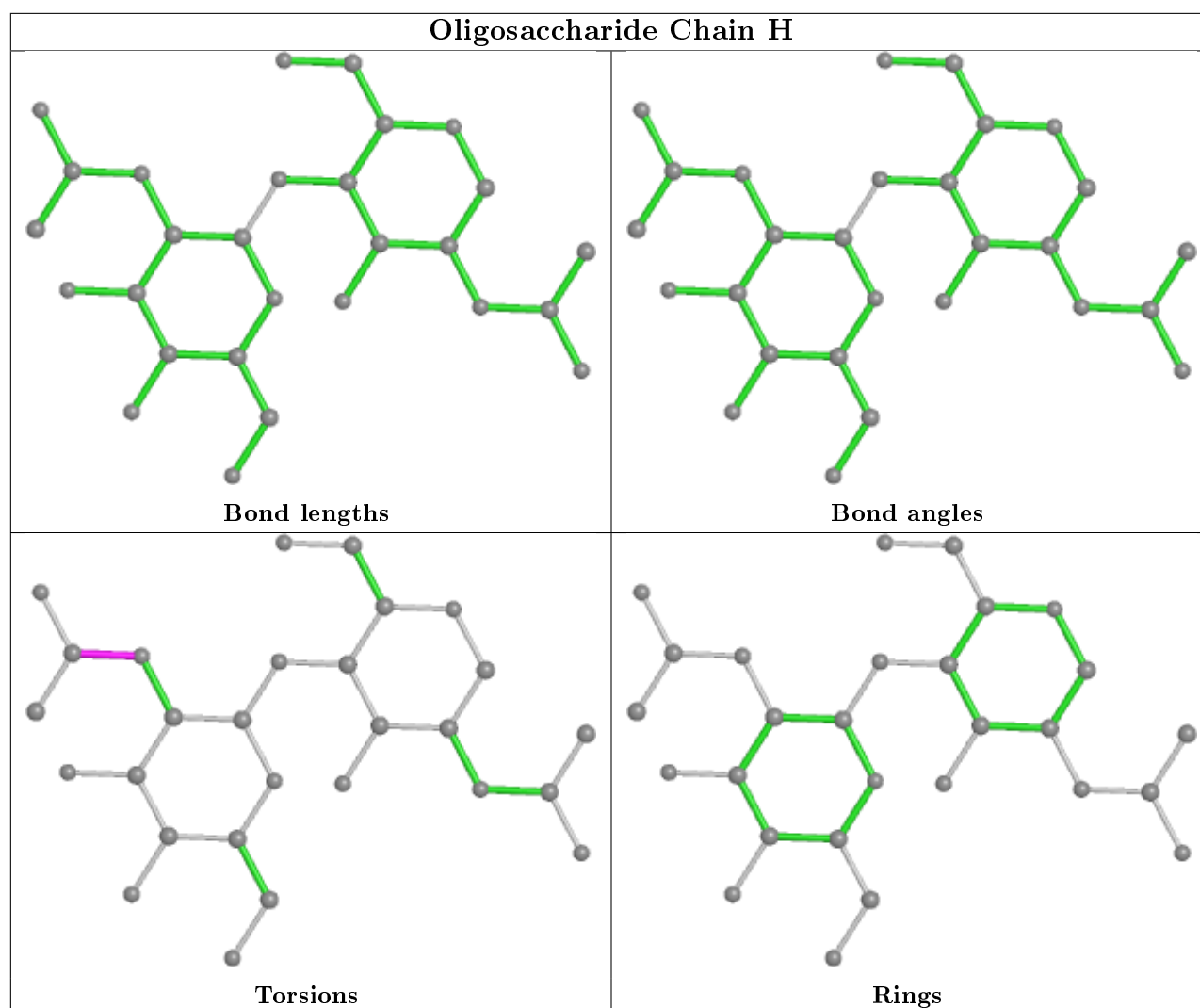
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	NAG	1	0
2	D	1	NAG	1	0
2	C	2	NAG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 10 are monoatomic - leaving 13 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	B	750	1	14,14,15	0.51	0	17,19,21	0.74	0
4	NAG	B	721	-	14,14,15	0.45	0	17,19,21	0.74	0
7	SO4	A	801	-	4,4,4	0.23	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	720	1	14,14,15	0.52	0	17,19,21	0.93	1 (5%)
4	NAG	A	720	1	14,14,15	0.49	0	17,19,21	0.86	0
4	NAG	A	750	1	14,14,15	0.57	0	17,19,21	0.55	0
4	NAG	B	760	1	14,14,15	0.51	0	17,19,21	0.73	0
4	NAG	A	721	-	14,14,15	0.47	0	17,19,21	0.69	0
7	SO4	B	800	-	4,4,4	0.27	0	6,6,6	0.07	0
7	SO4	A	800	-	4,4,4	0.26	0	6,6,6	0.06	0
4	NAG	A	700	1	14,14,15	0.51	0	17,19,21	0.66	0
4	NAG	B	700	1	14,14,15	0.53	0	17,19,21	0.60	0
4	NAG	A	760	1	14,14,15	0.55	0	17,19,21	0.67	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	721	-	-	2/6/23/26	0/1/1/1
4	NAG	A	760	1	-	4/6/23/26	0/1/1/1
4	NAG	B	720	1	-	0/6/23/26	0/1/1/1
4	NAG	A	720	1	-	0/6/23/26	0/1/1/1
4	NAG	A	750	1	-	4/6/23/26	0/1/1/1
4	NAG	B	760	1	-	4/6/23/26	0/1/1/1
4	NAG	A	721	-	-	2/6/23/26	0/1/1/1
4	NAG	A	700	1	-	4/6/23/26	0/1/1/1
4	NAG	B	700	1	-	4/6/23/26	0/1/1/1
4	NAG	B	750	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	720	NAG	C3-C4-C5	2.04	113.89	110.24
4	A	760	NAG	C2-N2-C7	-2.02	120.03	122.90

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	760	NAG	C8-C7-N2-C2
4	B	760	NAG	O7-C7-N2-C2
4	A	721	NAG	C8-C7-N2-C2
4	A	721	NAG	O7-C7-N2-C2
4	A	760	NAG	C8-C7-N2-C2
4	A	760	NAG	O7-C7-N2-C2
4	A	750	NAG	C8-C7-N2-C2
4	A	750	NAG	O7-C7-N2-C2
4	B	760	NAG	C4-C5-C6-O6
4	A	760	NAG	O5-C5-C6-O6
4	B	721	NAG	O5-C5-C6-O6
4	B	721	NAG	C4-C5-C6-O6
4	A	760	NAG	C4-C5-C6-O6
4	B	760	NAG	O5-C5-C6-O6
4	B	700	NAG	C8-C7-N2-C2
4	A	750	NAG	C4-C5-C6-O6
4	A	700	NAG	C8-C7-N2-C2
4	B	700	NAG	O7-C7-N2-C2
4	A	700	NAG	O5-C5-C6-O6
4	A	750	NAG	O5-C5-C6-O6
4	A	700	NAG	C4-C5-C6-O6
4	A	700	NAG	O7-C7-N2-C2
4	B	700	NAG	C4-C5-C6-O6
4	B	700	NAG	O5-C5-C6-O6
4	B	750	NAG	C4-C5-C6-O6
4	B	750	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	720	NAG	3	0
4	B	760	NAG	1	0
4	A	721	NAG	3	0
4	A	760	NAG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	559/559 (100%)	0.19	9 (1%) 72 70	8, 20, 31, 45	0
1	B	559/559 (100%)	0.27	7 (1%) 77 76	6, 21, 32, 44	0
All	All	1118/1118 (100%)	0.23	16 (1%) 75 74	6, 20, 32, 45	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	462	ALA	3.4
1	B	2	PRO	3.3
1	B	462	ALA	3.3
1	A	368	THR	2.7
1	A	463	VAL	2.6
1	B	315	ALA	2.6
1	A	555	ILE	2.5
1	A	31	GLY	2.5
1	A	314	GLY	2.5
1	A	68	ASN	2.5
1	B	3	THR	2.4
1	B	314	GLY	2.3
1	B	16	GLY	2.1
1	A	3	THR	2.1
1	B	319	LEU	2.0
1	A	325	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

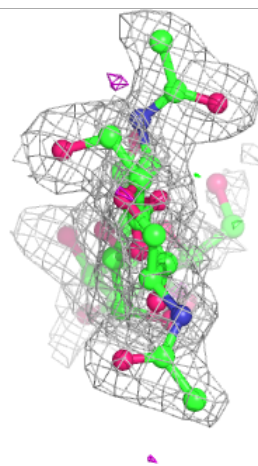
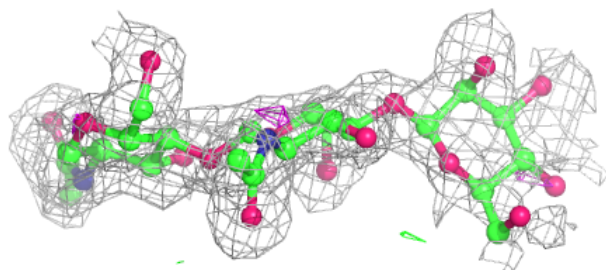
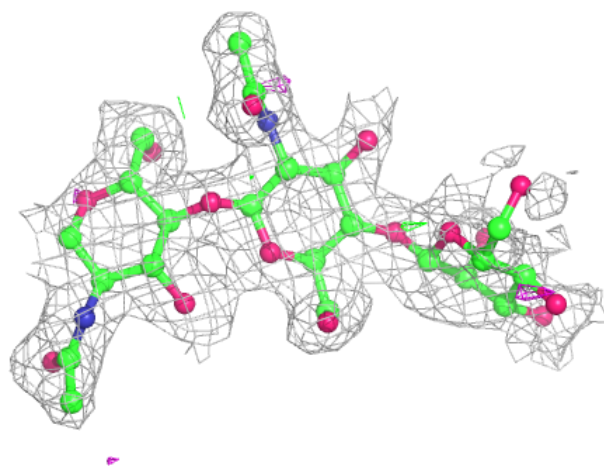
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BMA	F	3	11/12	0.59	0.30	47,50,54,55	0
2	BMA	D	3	11/12	0.63	0.25	42,45,48,49	0
2	BMA	C	3	11/12	0.69	0.31	43,48,52,54	0
3	NAG	H	2	14/15	0.73	0.29	41,43,44,46	0
2	BMA	G	3	11/12	0.73	0.29	43,48,50,51	0
3	NAG	H	1	14/15	0.79	0.16	30,32,34,38	0
2	NAG	G	2	14/15	0.79	0.20	24,30,33,39	0
3	NAG	E	2	14/15	0.81	0.30	41,46,49,49	0
3	NAG	E	1	14/15	0.82	0.15	25,30,33,37	0
2	NAG	D	2	14/15	0.85	0.14	24,26,30,37	0
2	NAG	C	2	14/15	0.88	0.15	12,24,30,36	0
2	NAG	F	2	14/15	0.90	0.11	23,29,34,40	0
2	NAG	D	1	14/15	0.90	0.11	15,18,22,22	0
2	NAG	C	1	14/15	0.90	0.14	18,22,23,23	0
2	NAG	F	1	14/15	0.90	0.12	20,21,23,24	0
2	NAG	G	1	14/15	0.91	0.11	19,22,24,24	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

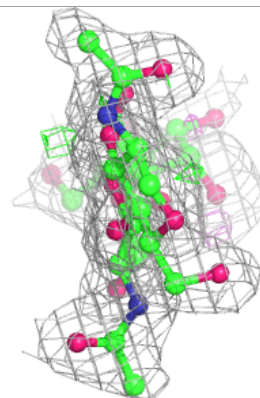
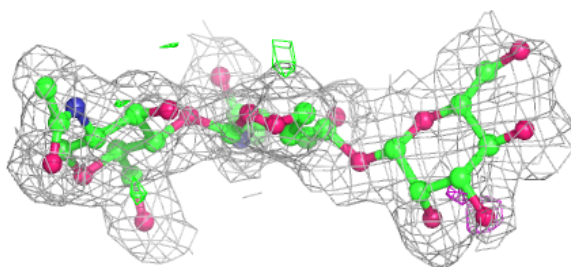
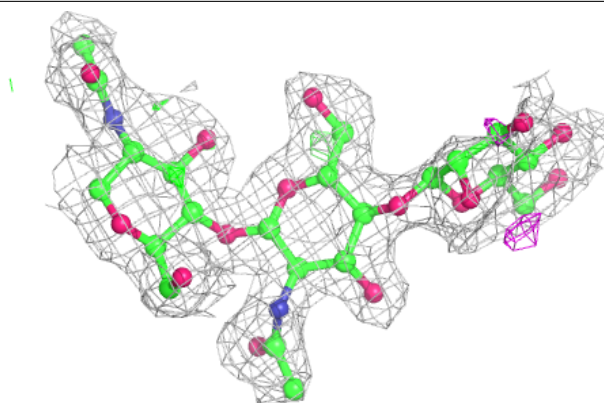
Electron density around Chain C:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

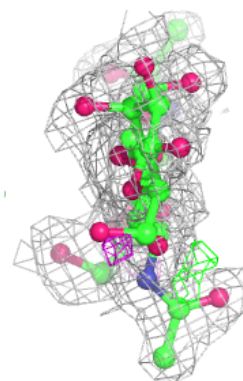
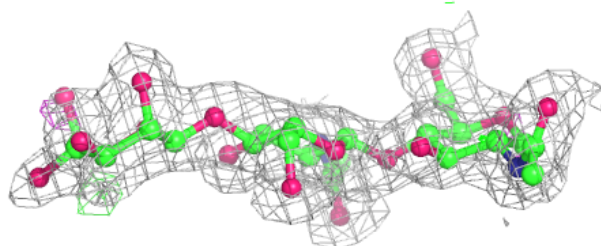
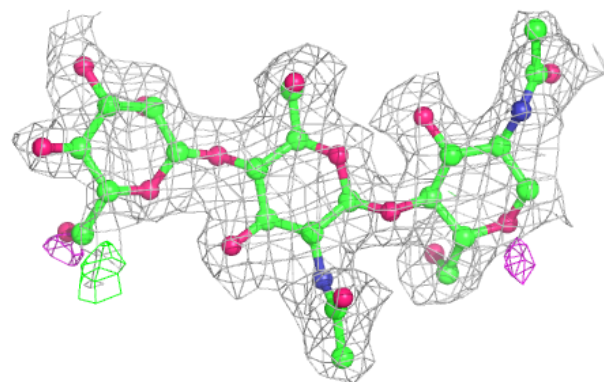


Electron density around Chain D:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

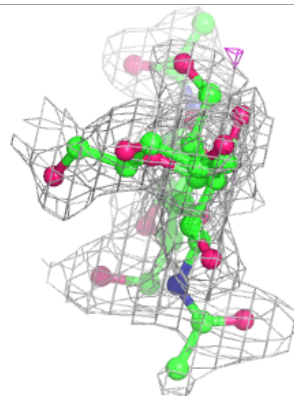
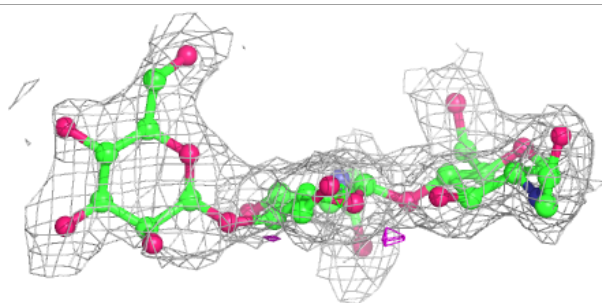
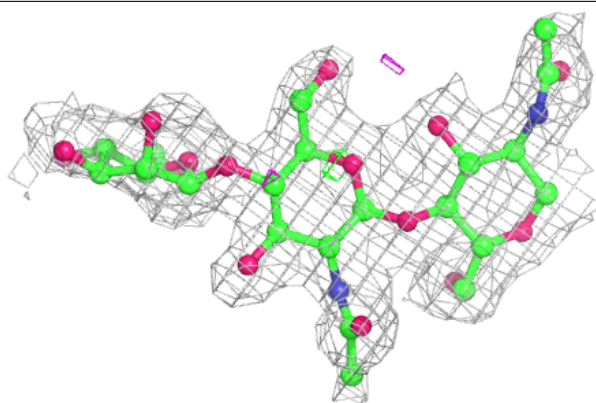
**Electron density around Chain F:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

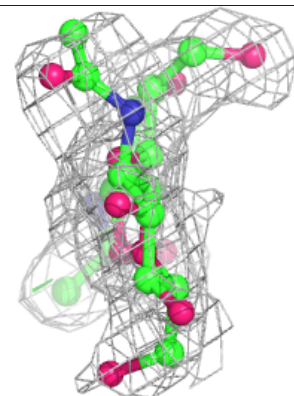
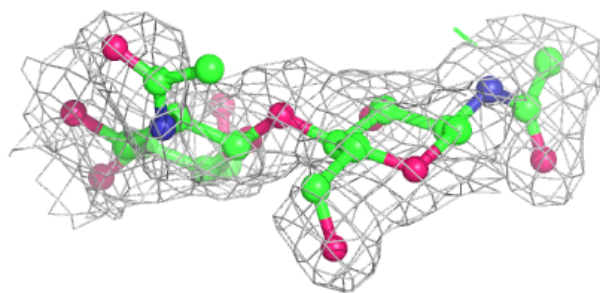
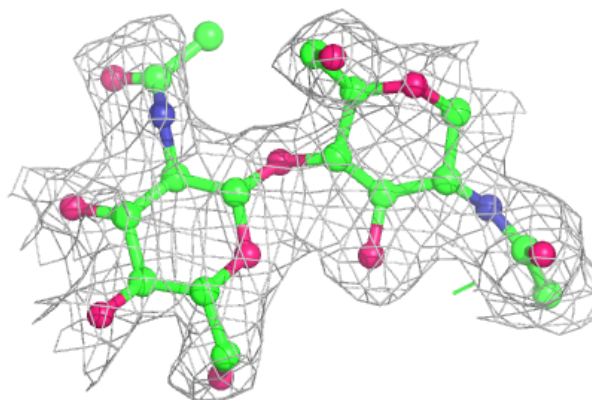


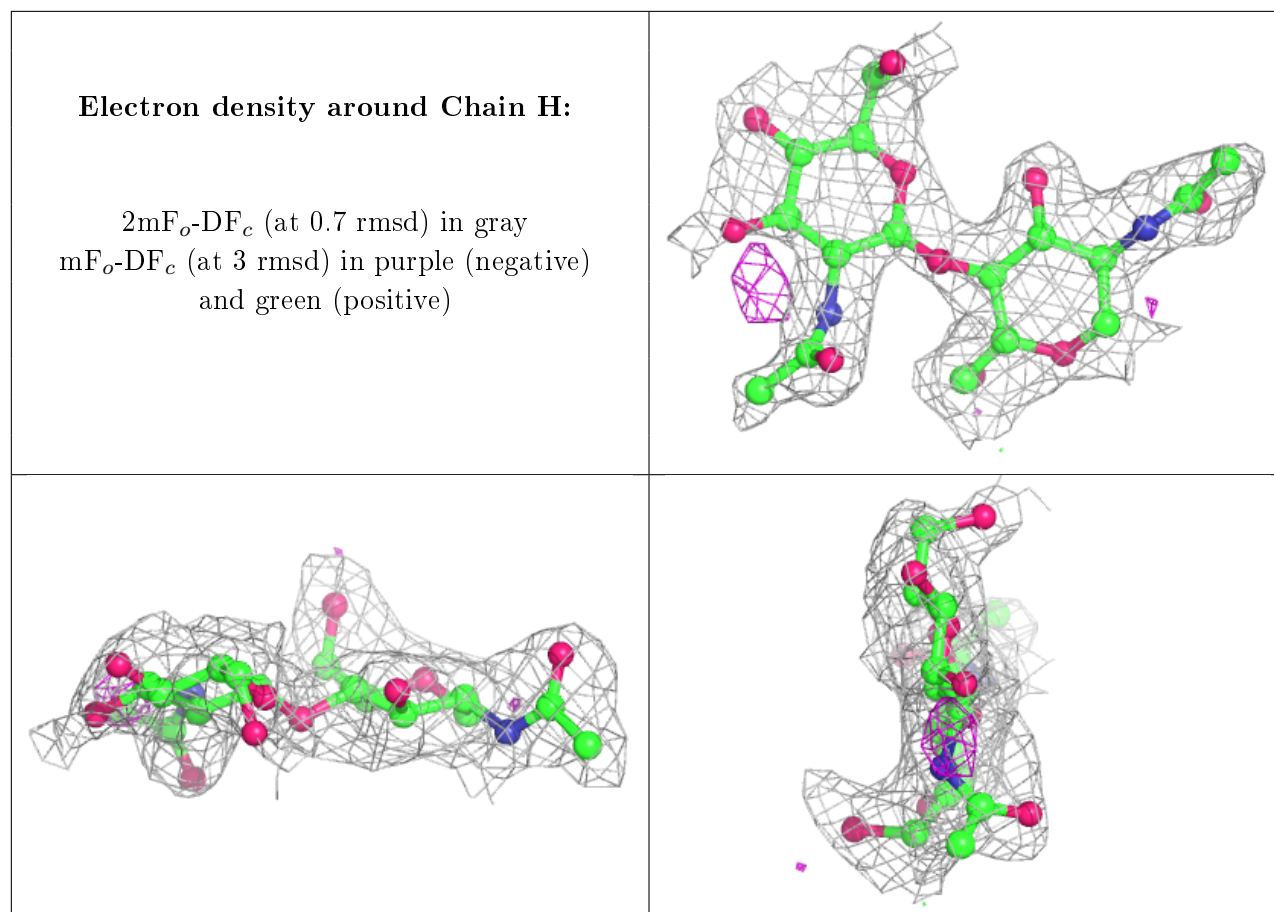
Electron density around Chain G:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain E:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	721	14/15	0.66	0.27	55,56,57,58	0
4	NAG	B	721	14/15	0.67	0.31	48,52,53,53	0
4	NAG	B	760	14/15	0.69	0.21	37,39,41,41	0
4	NAG	A	760	14/15	0.75	0.22	30,33,34,37	0
4	NAG	A	720	14/15	0.80	0.18	32,34,36,39	0
7	SO4	B	800	5/5	0.81	0.14	73,73,74,74	0
7	SO4	A	801	5/5	0.81	0.24	73,73,74,74	0
4	NAG	A	750	14/15	0.81	0.27	41,43,44,46	0
4	NAG	B	720	14/15	0.81	0.18	28,30,32,35	0
4	NAG	B	700	14/15	0.84	0.16	29,30,32,34	0
4	NAG	A	700	14/15	0.85	0.17	27,29,31,32	0
4	NAG	B	750	14/15	0.86	0.14	29,31,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	SO4	A	800	5/5	0.89	0.15	71,71,72,72	0
6	CL	B	610	1/1	0.95	0.13	32,32,32,32	0
6	CL	A	610	1/1	0.97	0.10	31,31,31,31	0
5	CU	B	601	1/1	0.98	0.04	17,17,17,17	0
5	CU	A	601	1/1	0.99	0.04	16,16,16,16	0
5	CU	A	602	1/1	0.99	0.02	19,19,19,19	0
5	CU	B	602	1/1	0.99	0.03	18,18,18,18	0
5	CU	A	603	1/1	1.00	0.04	16,16,16,16	0
5	CU	B	604	1/1	1.00	0.02	22,22,22,22	0
5	CU	A	604	1/1	1.00	0.03	21,21,21,21	0
5	CU	B	603	1/1	1.00	0.02	18,18,18,18	0

6.5 Other polymers ⓘ

There are no such residues in this entry.